
**CONDITIONS FOR THE MAXIMAL THERMOELECTRIC
POWER FACTOR YIELD IN INTERMETALLIC
SEMICONDUCTORS ZrNiSn AND TiCoSb****V.A. ROMAKA^{1,2}, D. FRUCHART³, YU.K. GORELENKO⁴,
YU.V. STADNYK⁴, L.P. ROMAKA⁴, M.G. SHELYAPINA⁵, V.F. CHEKURIN¹**UDC 621.315.592
©2006¹**Ya. Pidstryhach Institute of Applied Problems of Mechanics and Mathematics,
Nat. Acad. Sci. of Ukraine**
(3b, Naukova Str., Lviv 79060, Ukraine),²**National University "Lvivs'ka Politehnika"**
(12, Bandera Str., Lviv 79013, Ukraine; e-mail: vromaka@polynet.lviv.ua),³**Laboratoire de Cristallographie, CNRS**
(BP 166, Grenoble 38042, Cedex 9, France; e-mail: daniel.fruchart@grenoble.cnrs.fr),⁴**Ivan Franko Lviv National University**
(6, Kyryl and Mefodiy Str., Lviv 79005, Ukraine; e-mail: gorelenko_yuriy@franko.lviv.ua),⁵**V.A. Fock Institute of Physics of the St.-Petersburg National University**
(1, Ul'yanovskaya Str., Petrodvorets, St.-Petersburg 198504, Russia;
e-mail: marinashelyapinna@mail.ru)

The heavy doping of intermetallic semiconductors ZrNiSn and TiCoSb with acceptor and/or donor impurities up to the concentrations, at which the Fermi level becomes fixed at the mobility edge of the corresponding continuous energy band (the conduction or the valence one), has been shown to be a condition for obtaining the maximal thermoelectric power factor in these materials.

1 Introduction

In this work which continues our theoretical and experimental researches concerning the influence of the heavy doping of intermetallic semiconductors with a structure of the MgAgAs type by acceptor and/or donor impurities (N_A and $N_D \approx 10^{19} \div 10^{21} \text{ cm}^{-3}$) on their properties, the conditions for reaching the maximum of the thermoelectric power factor Z^* and keeping its thermal stability in ZrNiSn and TiCoSb semiconductors have been determined for the first time on the basis of the mechanisms of conductivity proposed by us earlier [1–7].

The earliest researches of intermetallic semiconductors have already demonstrated their capabilities as thermoelectric materials [8, 9]. The growing interest to undoped and doped intermetallic semiconductors is caused by high values of their conductivity σ and thermoelectric voltage α , which provides, in turn, considerable values for the thermoelectric power factor $Z^* = \alpha^2 \sigma$ and make them the most researched objects among new thermoelectric materials [1–12].

The analysis of works [1–12] revealed that, as a rule, only different techniques of doping and their combinations were tested in order to achieve the highest value of Z^* , without studying the mechanisms of conductivity in detail. In this context, we note the results of work [11], where the authors have reached the record values for Z^* in n -TiNiSn semiconductor doped with donor impurities by substituting Sn($4d^{10}5s^25p^2$) atoms for Sb($4d^{10}5s^25p^3$) ones. However, the mechanism of conductivity in TiNiSn $_{1-x}$ Sb $_x$ has not been determined in this work, and the regularities of the intermetallic semiconductor doping, which give rise to the maximal values of Z^* , remained obscure.

It should be noticed that, in the overwhelming majority of works known to us, the fabrication technology of the semiconductors concerned consisted in fusing the mixture of initial components followed by the uncontrollable cooling of the melt. In so doing, one of the ways to obtain disordered solids [13] is partially realized, but it brings about structure irregularities, local deformations of crystallites in polycrystalline specimens, and irregularities stimulated by the fluctuations in the considerable concentrations of charged impurities [14]. All that substantially influences the stability of the electrophysical properties of semiconductors.

Knowing the actual mechanisms of conductivity allows one not only to simulate but also to fabricate intermetallic semiconductors with a prescribed position of the Fermi level E_F by the proper choice of dopant concentrations, synthesis conditions, and regimes of homogenizing annealing and cooling, which would ultimately provide maximal values for Z^* in a wide range of temperatures. In addition, the issue of the semiconductor parameter stability in time at heat shocks, heat cycling, etc. is also of importance.

The calculations of electron structures and the experimental researches of the kinetic, magnetic, resonant, and structural characteristics of heavily doped and compensated intermetallic semiconductors n -ZrNiSn and p -TiCoSb enabled us to reveal the dominating mechanisms of conductivity in these semiconductors in wide temperature and concentration intervals, determine the role of impurity bands, and propose the models of the impurity band reconstruction under variations in the impurity concentration and the compensation factor [2–7]. The next logic step is to study the conditions for the maximum of the thermoelectric power factor in those semiconductors to be reachable and thermally stable. The presented paper is devoted to the solution of this task.

2 Experimental and Theoretical Methods

The behaviors of the specific electrical resistivity ρ , thermoelectric voltage α , magnetic susceptibility χ , and structural characteristics of the ZrNiSn and TiCoSb solid solutions were studied under doping them with various acceptor or donor impurities up to various impurity concentrations N_A and N_D (from $8.7 \times 10^{19} \text{ cm}^{-3}$ ($x = 0.005$) up to $5.7 \times 10^{21} \text{ cm}^{-3}$ ($x = 0.3$)). The following doping procedures were used:

1. Doping ZrNiSn with acceptor impurities by substituting Sc($3d^14s^2$) atoms for Zr($4d^25s^2$) ones (the formation of a $\text{Zr}_{1-x}\text{Sc}_x\text{NiSn}$ solid solution).

2. Doping TiCoSb with donor impurities by substituting Ni($3d^84s^2$) atoms for Co($3d^74s^2$) ones (the formation of a $\text{TiCo}_{1-x}\text{Ni}_x\text{Sb}$ solid solution).

3. Doping ZrNiSn with acceptor impurities by substituting Co atoms for Ni ones. In this variant, we studied both the tempered specimens (obtained by the gradual cooling to room temperature for 24 h after homogenizing annealing) and the hardened ones (fast cooling after annealing).

The methods of specimen fabrication and of measurement to determine the temperature dependences $\rho(T)$ and $\alpha(T)$ with respect to copper and $\chi(T)$ (the Faraday method) in the interval $T = 80 \div 380 \text{ K}$ were described in work [2]. The calculations of the corresponding electron structures were carried out in the framework of the self-consistent Korringa–Kohn–Rostoker (KKR) method, using the coherent potential (CPA) and local density (LDA) approximations [1, 3, 5, 7].

3 Results and Their Discussion

Figures 1 and 2 display the dependences of the thermoelectric power factor Z^* on the concentration of acceptor (the substitution of Sc atoms for Zr ones) and donor impurities in ZrNiSn and TiCoSb semiconductors, respectively. In the dependences $Z^*(x)$ for $\text{Zr}_{1-x}\text{Sc}_x\text{NiSn}$, one can observe a maximum in the vicinity of $x \approx 0.08$ indicated by the arrow. The position of the maximum almost does not depend on the temperature, being only slightly shifted towards larger values of Z^* at elevated temperatures.

The dependences $Z^*(x)$ for $\text{TiCo}_{1-x}\text{Ni}_x\text{Sb}$ are somewhat different from their analogs for $\text{Zr}_{1-x}\text{Sc}_x\text{NiSn}$. First, the maximum in the dependences $Z^*(x)$ manifests itself weakly; instead, an abrupt bend followed by the dependence $Z^*(x)$ becoming quasi-saturated at $x > 0.03$ is observed. Secondly, the right tail of the dependence $Z^*(x)$ little changes with the impurity concentration in the studied temperature interval.

Basing on the mechanisms of conductivity and the role of impurity bands in the conductivity of the given semiconductors [2–6], let us analyze the conditions for the maximum in the dependences $Z^*(x)$ to emerge.

While comparing the behavior of the dependences $Z^*(x)$ and $\alpha(x)$ [2–4] for $\text{Zr}_{1-x}\text{Sc}_x\text{NiSn}$, we notice that the maximum of the dependence $Z^*(x)$ is located in the downhill section of the dependence $\alpha(x)$ at the point that corresponds to the content $x \approx 0.08$, where its steepness is largest. As is shown in Figs. 2–4, it is in the vicinity of the content $x \approx 0.08$ that the hopping conduction over

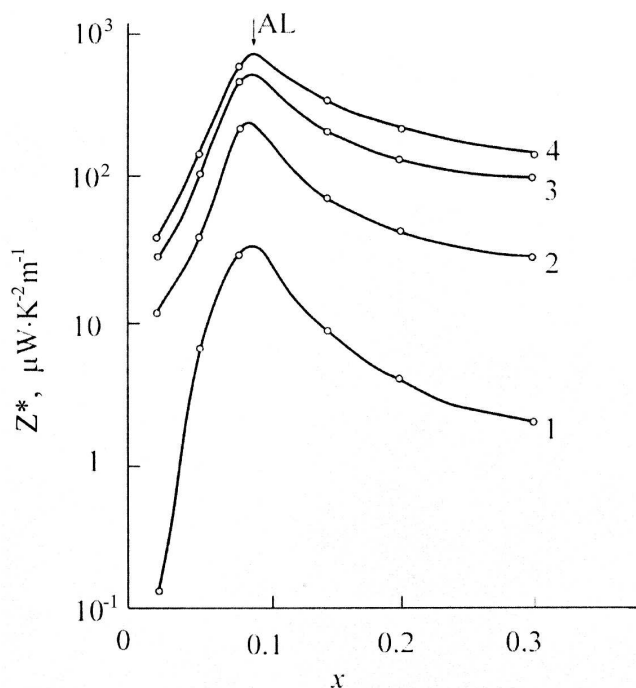


Fig. 1. Dependences $Z^*(x)$ of the thermoelectric power factor on the acceptor impurity concentration for $Zr_{1-x}Sc_xNiSn$ semiconductor at various temperatures $T = 80$ (1), 200 (2), 300 (3), and 375 K (4)

localized states with the energy ε_2 disappears, the energy of charge carrier activation from the Fermi level onto the level ε_1 in the valence band acquires the lowest value, and the Coulomb gap of the impurity band disappears. This concentration range is also the region, where the density of states at the Fermi level ($N(E_F)$) grows most quickly to become quasi-saturated afterwards and the electrical conductivity $\sigma(x)$ increases exponentially as the concentration of acceptor impurities rises owing to the increase of the concentration of free holes caused by the ionization of acceptors. We believe that, in the vicinity of the acceptor impurity concentration that corresponds to the content $x \approx 0.08$, the energy gap between the acceptor impurity band and the mobility edge of the valence band disappears, and the Fermi level becomes fixed by the latter.

At higher concentrations of acceptor impurities ($x > 0.1$), when the Fermi level enters the valence band and the transition insulator–metal is realized, the amplitude of the thermoelectric voltage decreases substantially. Since $Z^* = \alpha^2\sigma$, it is the behavior of the thermoelectric voltage that governs the behavior of the dependence $Z^*(x)$ in this concentration interval.

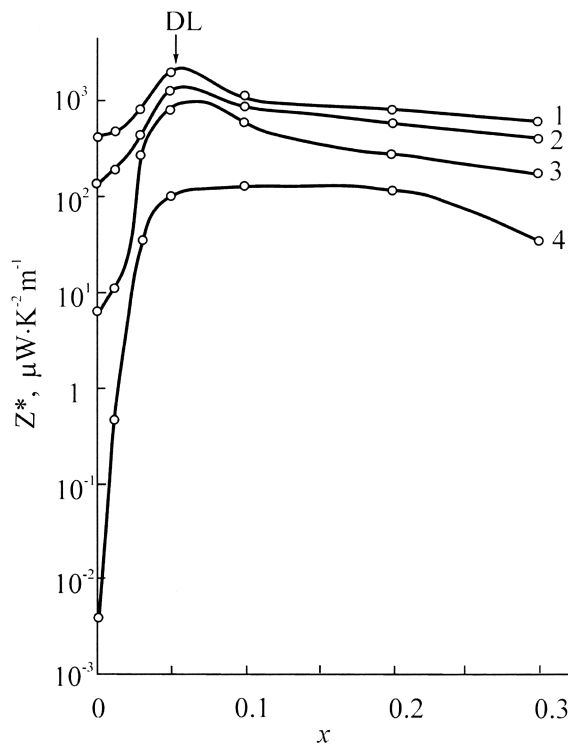


Fig. 2. The same as in Fig. 1 but for $TiCo_{1-x}Ni_xSb$

Summarizing the aforesaid, we can point out that the maximum of the thermoelectric power factor in the intermetallic $ZrNiSn$ semiconductors doped with acceptor impurities by means of substituting Sc atoms for Zr ones is observed at the impurity concentrations, at which the Fermi level becomes fixed at the mobility edge of the valence band. Therefore, the notation AL near the arrow in Fig. 1 means that the maximum is related to the acceptor impurity levels.

Concerning $TiCo_{1-x}Ni_xSb$ semiconductors, the quasi-saturation of the dependence $Z^*(x)$, after an insignificant maximum in it, is observed starting from the donor impurity concentration that corresponds to the content $x \approx 0.03$ (Fig. 2). By comparing the behavior of dependences $Z^*(x)$ and $\alpha(x)$ [5] for $TiCo_{1-x}Ni_xSb$, we notice that the maximum of the dependence $Z^*(x)$, similarly to the case of $Zr_{1-x}Sc_xNiSn$, is located in the downhill interval of the dependence $\alpha(x)$, at a point that corresponds to the content $x \approx 0.05$, where its steepness is largest.

The dependence $Z^*(x)$, especially in the vicinity of its maximum, similarly to the $Zr_{1-x}Sc_xNiSn$ case and following the same reasons, is better correlated

with the dependence of the thermoelectric voltage on the impurity concentration than with the electrical conductivity one. As is shown in [5], it is starting from the donor impurity concentration corresponding to the content $x \approx 0.03$ of the solid solution $\text{TiCo}_{1-x}\text{Ni}_x\text{Sb}$ that the hopping conduction over the impurity states in the donor band disappears, the activation of electrons from the Fermi level E_F onto the level ε_1 in the conduction band is not observed, the Coulomb gap in the donor impurity band disappears, the dependence $\sigma(x)$ changes its behavior, and the density of states at the Fermi level reaches its highest values and becomes quasi-saturated. We think that, in the vicinity of the donor impurity concentration that corresponds to the content $x \approx 0.05$, the energy gap between the donor impurity band and the mobility edge of the conduction band disappears, and the Fermi level becomes fixed at the latter.

At higher concentrations of donor impurities ($x > 0.05$), when the Fermi level enters into the conduction band and the insulator–metal transition is realized [13], an insignificant decrease of the thermoelectric voltage is observed, which determines the behavior of the dependence $Z^*(x)$.

Thus, the insignificant maximum of the thermoelectric power factor or its quasi-saturation, which depends on the donor impurity concentration in $\text{TiCo}_{1-x}\text{Ni}_x\text{Sb}$ (*DL* in Fig. 2), is observed at the impurity concentration that makes the position of the Fermi level fixed at the mobility edge of the conduction band.

In addition, we may conclude that the depth of the donor levels in the semiconductors relative to the edges of the continuous energy bands is shallower than the depth of the acceptor levels. This circumstance reveals itself in the different rates of the Fermi level displacement towards the continuous energy bands as the dopant concentration changes.

The case of the doping of intermetallic semiconductors ZrNiSn with acceptor impurities by substituting Co atoms for Ni ones is a little more difficult but more illustrative than the already considered cases. We recall that we investigated both tempered and hardened $\text{ZrNi}_{1-x}\text{Co}_x\text{Sn}$ specimens. In Figs. 3 and 4, the dependences of the thermoelectric power factor on the acceptor impurity concentration in ZrNiSn are depicted for the tempered and hardened specimens, respectively.

In the case of the tempered specimens, the dependences $Z^*(x)$ demonstrate maxima in the

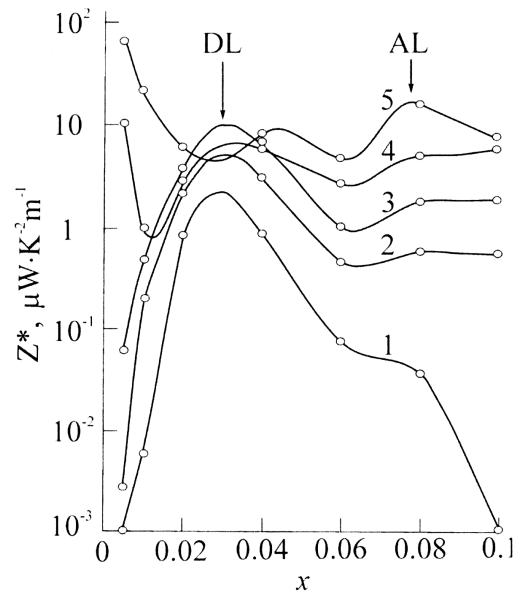


Fig. 3. Dependences $Z^*(x)$ for tempered $\text{ZrNi}_{1-x}\text{Co}_x\text{Sn}$ specimens at $T = 80$ (1), 150 (2), 200 (3), 300 (4), and 350 K (5)

temperature interval $T = 80 \div 300$ K for the acceptor impurity concentration that corresponds to the content $x \approx 0.03$. In addition, in the vicinity of the impurity concentration that corresponds to the content $x \approx 0.08$, a bend in the dependence $Z^*(x)$ is observed first (at $T = 80$ K). As the temperature grows, this bend is transformed into another maximum, whose position practically is not changed with temperature.

For the hardened specimens, the dependences $Z^*(x)$ also demonstrate maxima in the temperature interval $T = 80 \div 300$ K (Fig. 4). Nevertheless, at $T > 350$ K, a deep minimum (curve 5) replaces the first maximum in the dependence $Z^*(x)$. At the same time, the second maximum, whose position, similarly to the case of tempered specimens, is not changed with temperature, is observed in the vicinity of the content $x \approx 0.08$ of the $\text{ZrNi}_{1-x}\text{Co}_x\text{Sn}$ solid solution at all the investigated temperatures.

While comparing the behavior of the dependences $Z^*(x)$ and $\alpha(x)$ [7] for $\text{ZrNi}_{1-x}\text{Co}_x\text{Sn}$, we notice that the first maximum in the dependences $Z^*(x)$ is located in the uphill interval of the dependence $\alpha(x)$, at a point that corresponds to the content $x \approx 0.03$, where its steepness is largest.

In work [7], the mechanisms of conductivity in the intermetallic semiconductors concerned were established. It was also found that the investigated specimens contained impurities of two types: uncontrollable donor impurities and controllable

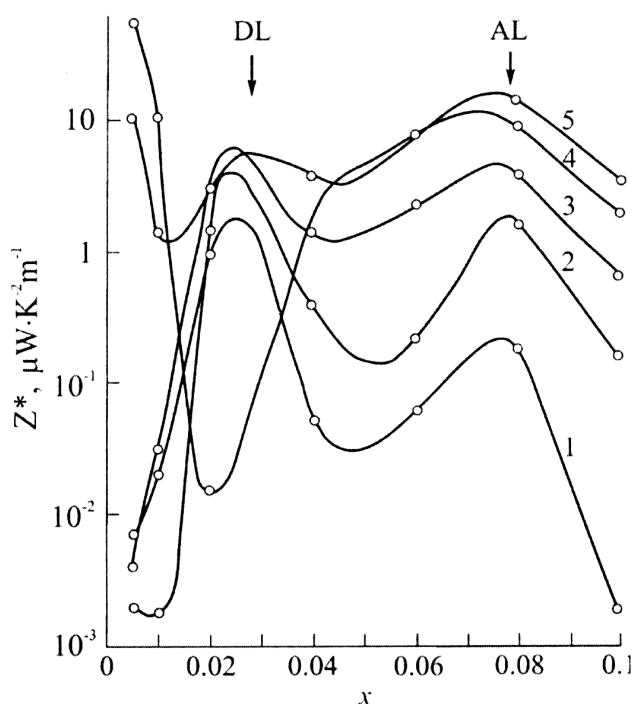


Fig. 4. The same as in Fig. 1 but for hardened $\text{ZrNi}_{1-x}\text{Co}_x\text{Sn}$ specimens

acceptor ones. The calculation of the density of states at the Fermi level in $\text{ZrNi}_{1-x}\text{Co}_x\text{Sn}$ showed, in its turn, that, in contrast to two cases considered above, the density of states changes nonmonotonously and there appears an additional maximum in the dependence of $N(E_F)$ on the impurity concentration.

In the interval of the acceptor impurity concentrations that correspond to the contents $0.005 \leq x \leq 0.03$, electrons are activated from the donor impurity band into the conduction one, and the activation energy decreases as the impurity concentration grows, which is characteristic of semiconductors with the electron type conductivity at their transition from the case of strong compensation ($1 - K \ll 1$) to the case of weak one ($K = N_A/N_D \ll 1$) [14].

The results of work [7] make it possible to determine how quickly the activation energy ε_1 changes in the interval $x \approx 0 \div 0.03$ of the acceptor impurity concentration: $d\varepsilon_1/dx \approx 240$ meV/at.%. The calculation shows that $\varepsilon_1 \approx 0$ at $x \approx 0.03$. It means that the Coulomb energy gap of the donor impurity band disappears at the acceptor impurity concentration which corresponds to the $\text{ZrNi}_{1-x}\text{Co}_x\text{Sn}$ content $x \approx 0.03$, and the impurity band merges with the mobility edge of the

conduction band, at which the position of the Fermi level becomes fixed. If the concentration of acceptor impurities increases and/or the temperature increases, which facilitates the ionization of acceptor impurities, the semiconductor becomes overcompensated from the n - to the p -type conductivity, with the Fermi level being now located in the Coulomb gap of the acceptor band. Whence, the disappearance of the maximum in the dependence $Z^*(x)$ at $T > 300$ K becomes clear.

Thus, the first maximum of the thermoelectric power factor in the intermetallic semiconductors ZrNiSn doped with acceptor impurities by substituting Co atoms for Ni ones is observed for the impurity concentration, at which the Fermi level turns out to be fixed at the mobility edge of the conduction band. The maximum in the dependence $Z^*(x)$ for $\text{TiCo}_{1-x}\text{Ni}_x\text{Sb}$ was, as we saw above, of a similar origin. We notice that the $\text{TiCo}_{1-x}\text{Ni}_x\text{Sb}$ semiconductor was doped with a donor impurity. Therefore, the donor impurity band is responsible for the maximum of the thermoelectric power factor, which makes it thermally stable in this compound. Since $\text{ZrNi}_{1-x}\text{Co}_x\text{Sn}$ was doped with an acceptor impurity and the first maximum is related with the donor impurity band (DL in Figs. 3 and 4), the first maximum for this compound is thermally unstable.

As for the second maximum observed at the acceptor impurity concentration that corresponds to the $\text{ZrNi}_{1-x}\text{Co}_x\text{Sn}$ content $x \approx 0.08$ in the dependences $Z^*(x)$, it is located in the downhill section of the dependences $\alpha(x)$ at the point of its largest steepness [7]. We have also found earlier [7] that, if the semiconductor has been overcompensated, a further increase of the acceptor impurity concentration leads to the reduction of the activation energy ε_1 and the Coulomb energy gap of the acceptor impurity band, followed by their disappearance, while the Fermi level drifts from the top of the acceptor impurity band to its bottom, and the density of states at the Fermi level reaches the highest values. At the acceptor impurity concentration that corresponds to the content $x \approx 0.08$, the acceptor impurity band and the mobility edge of the valence band overlap, and the Fermi level becomes fixed at the latter. At $x > 0.08$, the Fermi level enters into the interval of continuous energies in the valence band. That is, the insulator–metal transition is realized.

We may assert that the second maximum of the thermoelectric power factor in intermetallic semiconductors ZrNiSn (AL in Figs. 3 and 4) is observed for the impurity concentration, at which the position of the Fermi level becomes fixed at the mobility edge

of the valence band. Since this maximum is related to the acceptor impurity band, provided that the semiconductor is doped with acceptor impurities, it is thermally stable and only grows in the investigated temperature interval. In addition, while comparing Figs. 1, 3, and 4, one can see that the second maximum in the dependences $Z^*(x)$ for $\text{ZrNi}_{1-x}\text{Co}_x\text{Sn}$ and the maximum in $Z^*(x)$ for $\text{Zr}_{1-x}\text{Sc}_x\text{NiSn}$ are located at the identical concentrations of acceptor impurities and have the same origin: they are related to the Fermi level fixation at the mobility edge of the valence band.

To summarize the discussion, we pay attention to the behavior of the dependence $Z^*(x)$ for $\text{ZrNi}_{1-x}\text{Co}_x\text{Sn}$ at low (in these researches) concentrations of acceptor impurities ($x < 0.02$) and $T \geq 300$ K (curves 4 and 5 in Figs. 3 and 4). We believe that the drop of the quantity Z^* down by three orders of magnitude for some $\text{ZrNi}_{1-x}\text{Co}_x\text{Sn}$ specimens, when the variation of the acceptor impurity concentration in them corresponds to the variation of the content from $x = 0.05$ to $x = 0.02$, is caused by the cumulative action of the temperature and the impurity concentration on the Fermi level position. At $T \geq 300$, the Fermi level moves from the donor impurity band onto the mobility edge of the conduction band, and the capability to produce maximal yields of the thermoelectric power factor, which was declared above, becomes realized. As follows from Figs. 3 and 4, the maximal values of Z^* are attained just at $T \geq 300$ K, which is an extra argument for the conclusions made above.

Concerning the results of work [11], we would like to attract attention to the “arched” shape of the dependence $\rho(T)$ in TiNiSn with the maximum at $T \approx 170$ K (about 15 meV). Such a shape unequivocally testifies that, already in initial TiNiSn semiconductors still undoped with Sb, there is a considerable concentration of uncontrollable donor impurities, so that the conductivity over the donor impurity band has a metallic character rather than a hopping one (as we think, owing to the Mott-type insulator–metal transition [3, 13]). If $T > 170$ K, electrons are activated from the Fermi level in the impurity band into the conduction band, and ρ decreases as the temperature grows.

Doping TiNiSn with donor impurities to the concentration $N_D = 8.7 \times 10^{20} \text{ cm}^{-3}$, which corresponds to the semiconductor content $\text{TiNiSn}_{0.95}\text{Sb}_{0.05}$, and above gives rise to the disappearance of the activation section in the dependences $\rho(T)$. In our opinion, this fact can be explained by merging the donor impurity band and the mobility edge of the conduction band,

with the Fermi level being fixed at the latter, as was indicated above. The maximal values of the thermoelectric power factor were observed in work [11] just at $x = 0.05$. If the concentration of donor impurities is higher, the Fermi level will drift into the depth of the conduction band (we think that it is the insulator–metal transition of the Anderson type [3, 13]).

4 Conclusions

1. The heavy doping of intermetallic semiconductors ZrNiSn and TiCoSb with acceptor and/or donor impurities up to the impurity concentrations, at which the Fermi level E_F becomes fixed at the mobility edge of the corresponding continuous energy band, is a condition for the maximal yield of the thermoelectric power factor Z^* .
2. The maximum of the thermoelectric power factor is thermally stable, provided that the type of dopants which are introduced into the semiconductor and the type of the impurity band which is responsible for the appearance of the Z^* -maximum are of the same origin.
3. In $\text{Zr}_{1-x}\text{Sc}_x\text{NiSn}$ and $\text{ZrNi}_{1-x}\text{Co}_x\text{Sn}$ semiconductors, the acceptor impurity band formed by acceptor impurities of various types and the mobility edge of the valence band overlap at the same impurity concentration; this concentration corresponds to the content $x \approx 0.08$.
4. In $\text{TiCo}_{1-x}\text{Ni}_x\text{Sb}$ semiconductor, the donor impurity band and the mobility edge of the conduction band overlap at the donor concentration that corresponds to the content $x \approx 0.05$.

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УМОВИ ОТРИМАННЯ МАКСИМУМУ
КОЕФІЦІЄНТА ТЕРМОЕЛЕКТРИЧНОЇ
ПОТУЖНОСТІ В ІНТЕРМЕТАЛІЧНИХ
НАПІВПРОВІДНИКАХ ZrNiSn ТА TiCoSb

В.А. Ромака, Д. Фрушарт, Ю.К. Гореленко, Ю.В. Стадник,
Л.П. Ромака, М.Г. Шеляпіна, В.Ф. Чекурін

Резюме

Показано, що умовою отримання максимальних значень коефіцієнта термоелектричної потужності в інтерметалічних напівпровідниках ZrNiSn та TiCoSb є їх сильне легування акцепторними і/або донорними домішками до концентрацій, за яких рівень Фермі фіксується краєм рухливості відповідної зони неперервних енергій.